

1,1,2,3,3,3-Hexafluoro-2-(trifluoromethyl)propanesulphonic acid  
93762-09-5 | DTXSID90239569

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.41 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.37e-01

Confidence level: 6.23e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methylarsonic acid</div> <div>Measured: 1.83</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Monosodium methanearsonate</div> <div>Measured: 3.58</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>4-Methylbenzenesulfonic acid</div> <div>Measured: 3.60</div> <div>Predicted: 2.37</div>
<div>Image not found</div> <div>Methanesulfonic acid</div> <div>Measured: 10.4</div> <div>Predicted: 6.76</div>		